Numerical Simulation of Realistic Foam Microstructures

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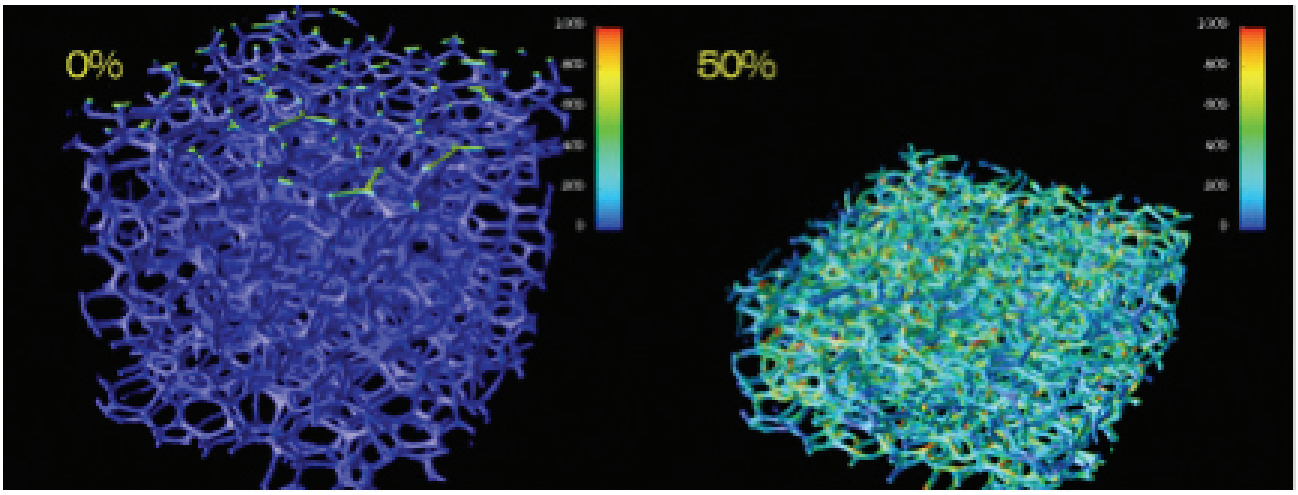
Foams are a class of material with unique properties and applications. They are lightweight and designed to undergo very large deformations. They are typically used in packaging and to absorb energy. Their properties are the result of the foam microstructure, a complex three-dimensional (3D) network of struts and, possibly, membranes, which undergo large deformations and contact during deformation. Foam deformation has been studied extensively and significant understanding has been obtained using idealized models. Experimental work has also served to demonstrate the complexity of foam deformation. However, as with other complex materials, developing a correspondence between characteristics of the microstructure and the bulk response is a grand challenge.

This scenario is fertile ground for numerical simulation but also a well-established computational challenge for several reasons. The reasons are: (1) the deformations of interest are large, both on average (macroscale) and on the microscale, (2) extensive "self-contact" must be simulated as the microstructure collapses, and (3) realistic foam microstructures, effectively a subject in rheology, are very complex and must be discretized. Recent developments in particle-in-cell (PIC) methods indicate that these numerical techniques are suitable for precisely this class of problem. Simulations have been performed that are extremely encouraging from several perspectives. Verification calculations have been performed to assess numerical accuracy in the simulation of quasistatic compression of homogeneous elastic material to 10% of its initial volume with good results. Macroscopic foam stress/strain curves agree qualitatively with experimental results and accepted model estimates of key deformation parameters. Simplified foam microstructures have been compressed to "full densification" and residual porosity studied, indicating incompressibility may not be a good assumption near full densification [1, 2].

Most recently, the compatibility of particle discretization and x-ray microtomography has been demonstrated. Figure 1 depicts an open cell foam microstructure obtained experimentally and discretized using a PIC method. The foam microstructure was obtained from Professor Gerald Seidler at the University of Washington (UW). The data are a 3D array of grey-scale values detailing relative x-ray cross-section. This data set was filtered to remove experimental artifacts and we used thresh-holding to improve contrast. The result is a regular array (voxels) with nonzero elements indicating the spatial position of material. The foam initial configuration was discretized by mapping from the voxels to a regular computational grid and placing polymer particles in computational cells for which the voxels indicate presence of material. The use of particles to generate the initial configuration provides a clear advantage over competing methods, where the generation of appropriate body fit meshes presents a formidable challenge.

Quasistatic compression of the foam microstructure was simulated using a PIC method. This run, to 90% compression, was done on the Linux cluster Grendels using 48 processors for about 300 hours. Of interest is the morphology of the deformed configurations as pore space is removed and the material is densified. Characterization of the deformed morphologies is a very challenging image-analysis task, which our collaboration with UW is also intended to address.

A connection between microstructural simulation and macroscopic (continuum) theory has also been sought. The development of macroscopic models of foam response is challenging. Existing models either determine the response of a specific microstructure and loading direction, or account for microstructure by scaling material parameters in more traditional, uniform continuum formulations. A new approach is under



development in which macroscopic response is determined from unit cell mechanics models and microstructural geometry statistics. These statistics are evolved throughout deformation. These simulations can provide precisely these data.

[1] S.G. Bardenhagen, A.D. Brydon, and J.E. Guilkey, "Insight into the Physics of Foam Densification via Numerical Simulation," *J. Mech. Phys. Solids* **53**, 3, 597 (2005).
[2] A.D. Brydon, et al., "Simulation of the Densification of Real Open-Celled Foam Microstructures," submitted to *J. Mech. Phys. Solids*.

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Acknowledgements
We would like to acknowledge NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program; and Campaign 2, Dynamic Materials Properties, for financial support.

Figure 1—
Realistic foam microstructure initial configuration (left) and simulated compressed state (right). Material is colored by a norm of the stress tensor.